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Research Paper

Metric Dimension for Line Graph of Some Chemical Structures

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Abstract

The metric dimension of a graph is a fundamental parameter that measures the minimum number of vertices to identify all other vertices in the graph uniquely. In the context of chemical structures, where graphs represent molecular entities, the metric dimension becomes a crucial metric for understanding molecular behavior and interactions. A subset $T = \{t_1, t_2, \ldots, t_k\}$ of nodes of a connected network G is referred to as a revolving set, if for any pair of nodes, $l, m \in V(G)$ there exists a node $t \in T$, such that its distances from l and m are different. The smallest cardinality of T is referred to as the metric dimension of G, and the nodes in T constitute a metric basis of G. In this work, we calculate the line graph's metric dimension for some chemical structures such as hexagon-square chains, linear phenylene structures, and linear heptagonal structures.

1 Introduction

In chemical graph theory, a collection of chemical compounds is mathematically defined in a way that provides different representations of various molecules. The idea of labeling graphs is used to represent the structure of a chemical compound whose node and line labels specify the atom and the bond respectively. Recent advances in mathematical chemistry provide a wide range of methods for tackling problems like understanding the underlying chemical structures of known chemical concepts, constructing and investigating new mathematical representations of chemical events, as well as applying mathematical techniques relevant to chemistry. Chemical graph theory, which is used to describe the structural characteristics of crystals, polymers,

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molecules, processes, clusters, and other entities, is a crucial field in mathematical chemistry. Further, mathematical chemistry recently presents a wide range of ways to deal with understanding the chemical structures that underlie existing chemical ideas, creating and researching novel mathematical models of chemical phenomena, and utilizing mathematical concepts and procedures in chemistry. In the pharmaceutical industry, finding new chemical structures for treating different diseases is affecting bigger development groups that comprise more broad and various synthetic endeavors targeted at increasingly complex activity spectra. These modifications are now being powered by fast technological advances in high-throughput screening combinatorial chemistry. The concept of metric dimension allows us to obtain a unique representation of chemical structures. In particular, they were used in pharmaceutical research to discover patterns common to a variety of drugs [1].

In chemistry, customary depictions of the structure of chemical compounds are graphs where the vertices and edges represent the atoms and bond types, respectively. The concept of metric dimension performs a significant role in the discovery of drugs, it is used to determine whether the features of a compound are responsible for its pharmacological activity, this idea is used in chemical compounds having similar structures (graph). Under the traditional view, we can determine whether any two compounds in the collection share the same functional group at a particular position. This comparative statement plays a critical role in drug discovery for determining whether the characteristics of a compound contribute to its pharmacological activity [2, 3].

The idea of metric dimension was first put forth by Slater in 1975 about difficulties with location[1] and it plays an important role in the development of medications since it may be used to assess whether a compound's characteristics cause its pharmacological activity. This notion is applied to chemical compounds with comparable structures [2, 3]. For efficient construction of massive data sets of a chemical structure [4], the notion of metric dimension is used. Metric dimensions are used in robot navigation [5], coin-weighing problems [6], computer networks [7], chemistry [2], combinatorial optimization [8], locating image processing facilities issues, sonar, and coastguard LORAN stations [1]. For different chemical structures represented by resolving parameters, we refer to [9].

In 2008, Indra et al. [7] determined that the metric dimension of honeycomb networks is 3. Shehnaz and Rashid [10] studied the metric dimension of the fullerene network. Min et al. [11] found the metric dimension of the line network $L(G)$ of G. Cyclic split networks' local metric dimension was derived by Cynthia and Ramya [12]. Henning et al. [13] studied computing the metric dimension for chain graphs. Ali et al. [14] examined the hollow coronoid's metric and fault-tolerant metric dimensions. Hamdon et al. [15] computed the generalized perimantanes diamondoid structure's vertex metric-based dimension. In 2021, Muhammad et al. [16] discovered the fault-tolerant metric dimension and metric dimension for various chemical structures.

We establish the metric dimensions for line graphs of specific chemical structures in this paper. Following is the arrangement of the remaining sections of the paper. Preliminaries and basic concepts are given in Section 2 and the main findings are detailed in Sections 3, 4, and 5. The implementation and applications of metric dimension in various fields and concluding remarks are in Sections 6 and 7 respectively.

2 Basis concepts

In this paper, connected, undirected, and finite graphs have been taken into consideration. They are also addressed as networks. A network is denoted also as $G = (V, E)$ where V is the set of nodes or vertices and E is the set of edges or lines in G. The distance $d(a,b)$ between any two nodes is the shortest (a,b)-path and is equal to the path's total number of edges. Let the collection of nodes at distance j from node x be denoted by $N_j(x)$.

Definition 2.1. A finite subset $T \subseteq V(G)$ of nodes is a locating or resolving set of G if, for every set of two vertices l, m in G, there exists a vertex $t \in T$ such that $d(l,t) \neq d(m,t)$. In other words, we say that $r(l|T) \neq r(m|T)$, where $r(x|T)$ is the identification of a node $g \in V(G)$ with respect to T, defined as $r(x|T) = (d(g,t_1), d(g,t_2), \ldots, d(g,t_k))$, where $T = \{t_1, t_2, \ldots, t_k\} \subseteq V$. A basis of G is the smallest resolving (locating) set, and its cardinality is denoted as $dim(G)$ and is referred to as the metric dimension of G.

Consider the graph G in Figure 1, for illustration. The set $W_1 = \{a_1, a_2\}$ is not a resolving set for G, since $r(a_7|W_1) = r(a_8|W_1) = r(a_9|W_1) = (4,3)$. Instead, $W_2 = \{a_1, a_2, a_7\}$ is a

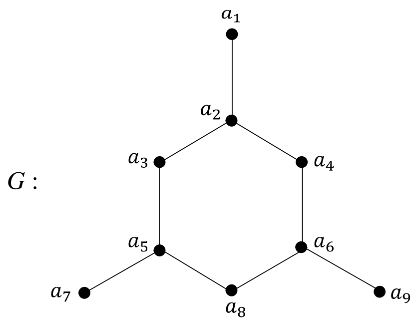

Figure 1

locating set for G. The identification of vertices with respect to W_2 are $r(a_1|W_2) = (0,1,4)$, $r(a_2|W_2) = (1,0,3)$, $r(a_3|W_2) = (2,1,2)$, $r(a_4|W_2) = (2,1,4)$, $r(a_5|W_2) = (3,2,1)$, $r(a_6|W_2) = (3,2,3)$, $r(a_7|W_2) = (4,3,0)$, $r(a_8|W_2) = (4,3,2)$ and $r(a_9|W_2) = (4,3,4)$. W_2 is not a smaller locating set, since $W_3 = \{a_1, a_7\}$ is also a resolving set. Since G cannot have a single vertex in its resolving, consequently W_3 is a minimum resolving set.

Definition 2.2. ([17]). Consider that $G = (V,E)$ is a connected, simple, and finite network. The line network of G, denoted by $L(G)$ is an undirected network in which $V(L(G)) = E$, and two distinct nodes are connected by an edge in $L(G)$ if and only if they are incident at the same vertex in G.

For illustration, a network G and its corresponding line network are shown in Figure 2.

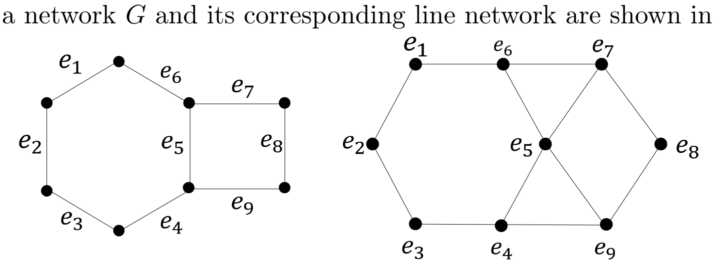

Figure 2: A network G and its line network $L(G)$.

The metric dimension for the line graph of a few chemical structures is determined in this section. We need the following results for our subsequent work.

Theorem 2.3. *([5]). Assume that the network $G = (V, E)$ has metric dimension 2 and let $\{x, y\} \subseteq V$ be a metric basis of G. Then, the following claims are valid.*

i) Between x and y, there is only one shortest path P.

ii) The maximum degree of each x and y is 3.

iii) Each of the internal nodes of P has a maximum degree of 5.

Theorem 2.4. *([3]). Suppose that G is a network of order $n \geq 2$. Then*

i) The metric dimension of graph G equals 1 if and only if G is a path network with n vertices.

ii) The metric dimension of graph G is $n - 1$ if and only if G is isomorphic to the complete graph K_n.

3 Main results

In chemical graph theory, the concept of metric dimension has found applications in understanding molecular structures, analyzing molecular graphs, chemical reactivity, bonding patterns, drug design, developing quantitative structure-activity relationships (QSAR), and so on. In this section, we obtain the metric dimension of the line graph of certain chemical architectures, such as cyclic hexagonal square chains, liner phenylene, and linear heptagonal structures.

3.1 Metric dimension of the line graph of cyclic hexagonal-square chain

A cyclic hexagonal-square chain [18] denoted by $C_{m,n}$ is a graph of molecules made up of m hexagonal chains that are mutually isomorphic H_1, H_2, $\ldots$, H_m, cyclically concatenated by circuits α_i of length 4, $1 \leq i \leq m$ in which $H_i s$ are chains containing m hexagons. In this paper, we consider $C_{1,n}$ where $m = 1$. For brevity, the graph $C_{1,n}$ is denoted by $C(n)$. For illustration, the cyclic hexagonal-square chain and it's corresponding line graph of dimension 5 are given in Figure 3.

We partition the vertices of $L(V(G))$ as I, O, and M, where I, O, and M are the set of all vertices in the inner cycle, outer cycle, and the middle vertices that are not on the inner and outer cycles respectively. The graph $L(C(n))$ is rotationally symmetric and has $8n$ vertices, in which $3n$ vertices are in each of the inner and outer cycles labeled as $O_1, O_2, \ldots, O_{3n}$ and $I_1, I_2, \ldots, I_{3n}$ in the clockwise direction respectively, and the remaining $2n$ middle vertices are labeled as $M_1, M_2, \ldots, M_{2n}$ in the clockwise direction as shown in Figure 4. The diameter of $L(C(n))$ is $\frac{3n+1}{2}$ when n is odd and $\frac{3n+2}{2}$ when n is even $n \geq 2$. Chemical and structural characteristics $L(C(n))$ are found in [18–20].

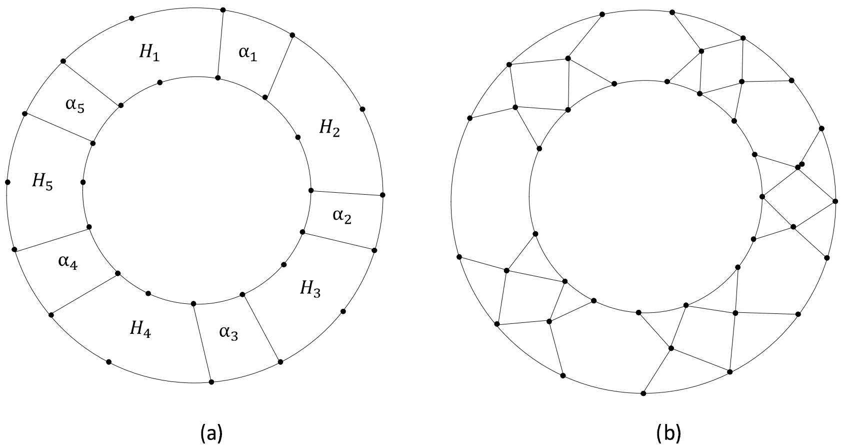

Figure 3: (a) Cyclic hexagonal-square chain of dimension 5, (b) Line graph of cyclic hexagonal-square chain of dimension 5.

Theorem 3.1. *Let G be a cyclic hexagonal-square chain $C(n)$. Then $dim(L(G)) \geq 3$, for $n \geq 2$.*

Proof. Suppose $L(G)$ has a metric basis equal to 2. Let $W = \{x, y\}$ be a metric basis of $L(G)$.

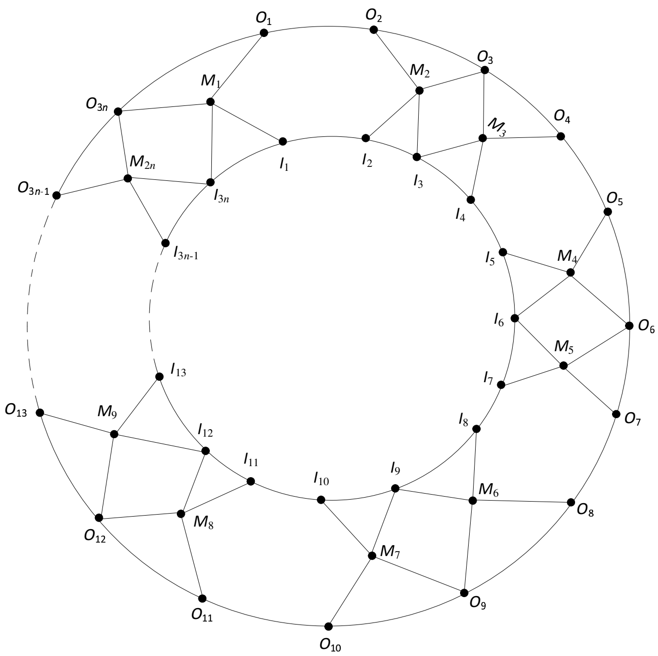

Figure 4: The labeling of the line network of a cyclic hexagonal-square chain of dimension n.

Case 1 (n is odd): The following subcases are now available.
Case 1(a): Both x and y are in I.

For $2 \leq j \leq \frac{3n-1}{2}$, if $W = \{O_1, O_j\}$ is a locating set, then $r(O_{3n-1}|W) = r(M_{2n}|W) = (2, j+1)$.
For $j = \frac{3n-1}{2} + 1$, if $W = \{O_1, O_j\}$ is a locating set, then $r(O_{3n-1}|W) = r(M_2|W) = (2, j-2)$.
For $j = \frac{3n-1}{2} + 2$, if $W = \{O_1, O_j\}$ is a locating set, then $r(I_{3n}|W) = r(M_2|W) = (2, j-2)$.
For $j = \frac{3n-1}{2} + 3$, if $W = \{O_1, O_j\}$ is a locating set, then $r(I_1|W) = r(O_3|W) = (2, j-3)$.
For $\frac{3n-1}{2} + 4 \leq j \leq 3n$, if $W = \{O_1, O_j\}$ is a locating set, then $r(O_3|W) = r(M_2|W) = (2, 3n - j + 3)$. Thus, the set W chosen is not a metric basis for any of the above cases.

Since the graph is rotationally symmetric, considering any two vertices in O is the same as that of I.

Case 1(b): Suppose $x \in I$ and $y \in O$. The resolving set between the outer and inner cycle is as follows.
If $W = \{O_1, I_1\}$ is a resolving set, then $r(M_{2n}|W) = r(M_2|W) = (2, 2)$.
For $2 \leq j \leq \frac{3n-1}{2} + 1, j \equiv 1,\ 2\ (mod\ 3)$ if $W = \{O_1, I_j\}$ is a resolving set, then $r(I_{\frac{3n-1}{2}+2}|W) = r(M_{n+1}|W) = (\frac{3n+1}{2}, \frac{3n+3-2j}{2})$.
For $\frac{3n-1}{2} + 3 \leq j \leq 3n - 1, j \equiv 1,\ 2\ (mod\ 3)$ if $W = \{O_1, I_j\}$ is a resolving set, then $r(I_{\frac{3n-1}{2}+2}|W) = r(M_{n+1}|W) = (\frac{3n+1}{2}, \frac{2j-3n-1}{2})$.
The case when $x \in I$ and $y \in O$ can be dealt with similarly.

The cases when (i) $x, y \in M$, (ii) $x \in I$, $y \in M$, and (iii) $x \in M$, $y \in I$, (iv) $x \in M$, $y \in O$, and $x \in O$, $y \in M$ are all ruled out by Theorem 2.3 as at least one of them would have degree 4.

Case 2 (n is even): Now we have the following subcases.
Case 2(a): Suppose both x and y are in O.
For $1 \leq j \leq \frac{3n}{2}$. if $W = \{O_1, O_j\}$ is a locating set of $L(G)$, then $r(O_{3n-1}|W) = r(M_{2n}|W) = (2, j+1)$.
For $\frac{3n}{2} + 3 \leq j \leq 3n$ let $W = \{O_1, O_j\}$ be a locating set, then $r(O_3|W) = r(M_2|W) = (2, 3n - j + 3)$.
For $j = \frac{3n}{2} + 1$, let $W = \{O_1, O_j\}$ is a locating set, then $r(M_{2n}|W) = r(M_2|W) = (2, j-2) = (2, 5)$.
For $j = \frac{3n}{2} + 2$, let $W = \{O_1, O_j\}$ is a locating set, then $r(I_{3n}|W) = r(O_3|W) = (2, j-3)$. Thus, the set W chosen is not a metric basis for any of the above cases.
Since the graph is rotationally symmetric, considering any two vertices in O is the same as that of I.
Case 2(b): Suppose $x \in I$ and $y \in O$ are in $L(G)$. The resolving set between the outer and inner cycle is as follows.
For $j = 1$, if $W = \{O_1, I_j\}$ is a locating set then $r(M_{2n}|W) = r(M_2|W) = (2, 2)$.
For $j = 2$, if $W = \{O_1, I_j\}$ is a locating set then $r(I_{3n-1}|W) = r(O_4|W) = (3, 3)$.
For $3 \leq j \leq \frac{3n}{2} + 2$, if $W = \{O_1, I_j\}$ is a locating set then $r(I_{\frac{3n}{2}+2}|W) = r(M_{n+2}|W)$.
For $\frac{3n}{2} + 3 \leq j \leq 3n$, if $W = \{O_1, I_j\}$ is a locating set then, $r(M_{\frac{3n}{2}+2}|W) = r(M_{n+1}|W)$.
Let $W = \{O_2, I_j\}$ is mirror image of $\{O_1, I_j\}$ and rotationally symmetric.
The cases when $x \in I$ and $y \in O$ can be dealt with similarly.
The cases when (i) $x, y \in M$, (ii) $x \in I$, $y \in M$, and (iii) $x \in M$, $y \in I$, (iv) $x \in M$, $y \in O$, and $x \in O$, $y \in M$ are all ruled out by Theorem 2.3 as at least one of them would have degree 4.
Hence, in both cases, we conclude that $dim(L(G)) \geq 3$. ■

Theorem 3.2. *Let G be a cyclic hexagonal-square chain $C(n)$. Then $dim(L(G)) = 3$, $n \geq 2$.*

Proof. By Theorem 3.1, we have $dim(L(G)) \geq 3$. We will prove the equality with the subsequent two cases.
Case 1 (n is odd): We claim that $W = \{O_1, O_{\frac{3n-1}{2}}, O_{3n-1}\}$ is a resolving set of $L(C_{m,n})$. It is enough to prove that, $N_j(O_1) \cap N_j(O_{\frac{3n-1}{2}}) \cap N_j(O_{3n-1}) = 0$ *or* 1, where $j \in \{1, 2, 3, \ldots, \frac{3n+1}{2}\}$.

For any j, $1 \leq j \leq \frac{3n-1}{2}$ the j^{th} neighbourhood of O_1 is given by $N_j(O_1) = \{O^j, M^j, I^j\}$, where

$$O^j = \begin{cases} \{O_{3n}, O_2\}, & \text{if } j = 1, \\ \{O_{j+1}, O_{3n+1-j}\}, & \text{if } 2 \leq j \leq \frac{3n-1}{2}, \end{cases}$$

$$M^j = \begin{cases} M_{\frac{2j}{3}+1}, & \text{if } j \equiv 0 \ (mod\ 3),\ j < \frac{3n+1}{2}, \\ M_j, & \text{if } j = 1, \\ M_{\frac{6n-2j+5}{3}}, & \text{if } j \equiv\ 1 (mod\ 3),\ j \neq 1, \text{ and } j < \frac{3n+1}{2}, \\ \{M_{2n-2(\frac{j+1}{2}+2)}, m_{2\frac{j+1}{3}}\}, & \text{if } j \equiv\ 2\ (mod\ 3)\ and\ j < \frac{3n+1}{2}, \\ M_{n+1}, & \text{if } j = \frac{3n+1}{2}, \end{cases}$$

$$I^j = \begin{cases} \{I_{3n}, I_{j-1}\}, & \text{if } j = 2, \\ \{I_{3n-j}, I_{j-1}, I_{j+1}\}, & \text{if } j = 3, \\ I_{3n-j+2}, & \text{if } 4 \leq j \leq \frac{3n+1}{2}. \end{cases}$$

For any j, $1 \leq j \leq \frac{3n-1}{2}$ the j^{th} neighbourhood of $O_{\frac{3n-1}{2}}$ is given by $N_j(O_{\frac{3n-1}{2}}) = \{O^j, M^j, I^j\}$, where

$$O^j = \begin{cases} \{O_{\frac{3n-1+2j}{2}}, O_{\frac{3n-2j-1}{2}}\}, & \text{if } 1 \leq j \leq \frac{3n-3}{2}, \\ \{O_{3n-1}, O_{3n}\}, & \text{if } j = \frac{3n-1}{2}, \end{cases}$$

$$M^j = \begin{cases} M_{\frac{2j}{3}+n}, & \text{if } j \equiv\ 0\ (mod\ 3),\ j < \frac{3n+1}{2}, \\ M_n, & \text{if } j = 1, \\ M_{\frac{3n-2j+2}{3}}, & \text{if } j \equiv\ 1\ (mod\ 3),\ j \neq 1\ and\ j < \frac{3n+1}{2}, \\ \{M_{\frac{3n+2j-1}{3}}, M_{\frac{3n-2j+1}{3}}\}, & \text{if } j \equiv\ 2\ (mod\ 3),\ j < \frac{3n+1}{2}, \\ M_{2n}, & \text{if } j = \frac{3n+1}{2}, \end{cases}$$

$$I^j = \begin{cases} \{I_{\frac{3n-1}{2}}, I_{\frac{3n-3}{2}}\}, & \text{if } j = 2, \\ \{I_{\frac{3n+3}{2}}, I_{\frac{3n+1}{2}}, I_{3n-5}\}, & \text{if } j = 3, \\ \{I_{\frac{3n+2j-3}{2}}, I_{\frac{3n-2j+1}{2}}\}, & \text{if } 4 \leq j \leq \frac{3n-1}{2}, \\ \{I_{3n}, I_{3n-1}\}, & \text{if } j = \frac{3n+1}{2}. \end{cases}$$

For any j, $1 \leq j \leq \frac{3n-1}{2}$, the j^{th} neighbourhood $N_j(O_{3n})$ is given by $N_j(O_{3n}) = \{O^j, M^j, I^j\}$, where

$$O^j = \begin{cases} \{O_{3n}, O_{3n-2}\}, & \text{if } j = 1, \\ \{O_{j-1}, O_{3n-j-1}\}, & \text{if } 2 \leq j \leq \frac{3n-1}{2}, \end{cases}$$

$$M^j = \begin{cases} M_{\frac{6n-2j}{3}}, & \text{if } j \equiv\ 0\ (mod\ 3),\ j < \frac{3n+1}{2}, \\ M_{2n}, & \text{if } j = 1, \\ M_{\frac{2j-2}{3}}, & \text{if } j \equiv\ 1\ (mod\ 3),\ j \neq 1\ and\ j < \frac{3n+1}{2}, \\ \{M_{\frac{2j-1}{3}}, m_{\frac{6n-2j+1}{3}}\}, & \text{if } j \equiv\ 2\ (mod\ 3),\ j < \frac{3n+1}{2}, \\ M_j, & \text{if } j = \frac{3n+1}{2}, \end{cases}$$

$$I^j = \begin{cases} \{I_{3n}, I_{3n-1}\}, & \text{if } j = 2, \\ \{I_{j-2}, I_{3n-3}, I_{3n-2}\}, & \text{if } j = 3, \\ \{I_{j-2}, I_{3n-j}\}, & \text{if } 4 \leq j \leq \frac{3n+1}{2}. \end{cases}$$

Case 2 (n is even):

Let $W = \{O_1, O_2, O_{\frac{3n+2}{2}}\}$ be a locating set of $L(C_{m,n})$. To prove W is a locating set it is enough to prove $N_j(O_1) \cap N_j(O_2) \cap N_j(O_{\frac{3n+2}{2}}) = 0$ *or* 1, where $j \in \{1, 2, 3, \ldots, \frac{3n+2}{2}\}$.
For any j, $1 \leq j \leq \frac{3n}{2}+1$ the j^{th} neighbourhood of O_1 is given by $N_j(O_1) = \{O^j, M^j, I^j\}$, where

$$O^j = \begin{cases} \{O_{3n+1-j}, O_{j+1}\}, & \text{if } 1 \leq j \leq \frac{3n}{2}, \\ O_{j+1}, & \text{if } j = \frac{3n}{2}+1, \end{cases}$$

$$M^j = \begin{cases} M_j, & \text{if } j = 1, \\ \{M_{\frac{6n-2j+4}{3}}, M_{\frac{2y+2}{3}}\}, & \text{if } j \equiv 2 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ M_{\frac{2j+3}{3}}, & \text{if } j \equiv 3 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ M_{\frac{6n-2j+5}{3}}, & \text{if } j \equiv 1 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ \{M_{2n-2(\frac{j+1}{2}+2)}, M_{2(\frac{j+1}{3})}\}, & \text{if } j \equiv 2 \ (mod\ 3), \quad j \leq \frac{3n+1}{2}, \\ M_{n+1}, & \text{if } j = \frac{3n}{2}, \end{cases}$$

$$I^j = \begin{cases} \{I_{3n}, I_{j-1}\}, & \text{if } j = 2, \\ \{I_{3n-1}, I_{j-1}, I_j\}, & \text{if } j = 3, \\ \{I_{3n-j+2}, I_j\}, & \text{if } 4 \leq j \leq \frac{3n}{2}, \\ I_j, & \text{if } j = \frac{3n}{2}+1. \end{cases}$$

For any j, $1 \leq j \leq \frac{3n}{2}+1$ the j^{th} neighbourhood of O_2 is given by $N_j(O_2) = \{O^j, M^j, I^j\}$, where

$$O^j = \begin{cases} \{O_j, O_{j+2}\}, & \text{if } j = 1, \\ \{O_{3n+2-j}, O_{j+2}\}, & \text{if } 2 \leq j \leq \frac{3n}{2}-1, \\ O_{j+2}, & \text{if } j = \frac{3n}{2}, \end{cases}$$

$$M^j = \begin{cases} M_{j+1}, & \text{if } j = 1, \\ \{M_{j-1}, M_{j+1}\}, & \text{if } j = 2, \\ \{M_{\frac{2j+5}{3}}, M_{\frac{6n-2j+1}{3}+2}\}, & \text{if } j \equiv 2 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ M_{\frac{6n-2j+6}{3}}, & \text{if } j \equiv 3 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ M_{\frac{2j+4}{3}}, & \text{if } j \equiv 1 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ M_{n+2}, & \text{if } j = \frac{3n}{2}; \end{cases}$$

$$I^j = \begin{cases} \{I_j, I_{j+3}\}, & \text{if } j = 2, \\ \{I_{3n}, I_{j-2}, I_{j+1}\}, & \text{if } j = 3, \\ \{I_{3n+3-j}, I_{j+1}\}, & \text{if } 4 \leq j \leq \frac{3n}{2}, \\ I_{j+1}, & \text{if } j = \frac{3n}{2}+1. \end{cases}$$

For any j, $1 \leq j \leq \frac{3n}{2}+1$, the j^{th} neighbourhood of $O_{\frac{3n+2}{2}}$ is given by $N_j(O_{\frac{3n+2}{2}}) = \{O^j, M^j, I^j\}$, where

$$O^j = \begin{cases} \{O_{\frac{3n+2j+2}{2}}, O_{\frac{3n+2-2j}{2}}\}, & \text{if } 1 \leq j \leq \frac{3n}{2}-1, \\ O_1, & \text{if } j = \frac{3n}{2}, \end{cases}$$

$$M^j = \begin{cases} M_{n+1}, & \text{if } j = 1, \\ \{M_{\frac{3n-2j+4}{3}}, M_{\frac{3n+2j+2}{3}}\}, & \text{if } j \equiv 2 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ M_{\frac{3n+2j+3}{3}}, & \text{if } j \equiv 3 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ M_{\frac{3n-2j+5}{3}}, & \text{if } j \equiv 1 \ (mod\ 3), \quad j < \frac{3n}{2}, \\ M_1, & \text{if } \quad j = \frac{3n}{2}, \end{cases}$$

$$I^j = \begin{cases} \{I_{\frac{3n+2}{2}}, I_{\frac{3n}{2}}\}, & \text{if } j = 2, \\ \{I_{\frac{3n+6}{2}}, I_{\frac{3n+4}{2}}, I_{\frac{3n-2}{2}}\}, & \text{if } j = 3, \\ \{I_{\frac{3n+2j}{2}}, I_{\frac{3n-2j+2}{2}}\}, & \text{if } 4 \leq j \leq \frac{3n}{2}, \\ I_1, & \text{if } j = \frac{3n}{2} + 1. \end{cases}$$

Thus, by the above discussion, it is clear that for n is odd $N_j(O_1) \cap N_j(O_{\frac{3n-1}{2}}) \cap N_j(O_{3n-1}) = 0 \ or \ 1$, and for n is even $N_j(O_1) \cap N_j(O_2) \cap N_j(O_{\frac{3n+2}{2}}) = 0 \ or \ 1$. Hence the metric dimension of $L(G)$ is 3. ■

4 Metric dimension for line graph of phenylene structure

The linear phenylene structure of dimension n, denoted by PS_n, consists of n alternating rhombuses and hexagonal rings that are connected to one another by bicyclo propene units, see Figure 5. The labeling of the line graph of the linear phenylene structure is given in Figure 6. It has 3 levels, top, middle, and bottom. Label the vertices in the top, middle, and bottom as $a_1, a_2, \ldots, a_{3n-1}$; $b_1, b_2, \ldots, b_{2n}$; and $c_1, c_2, \ldots, c_{3n-1}$ from left to right respectively.

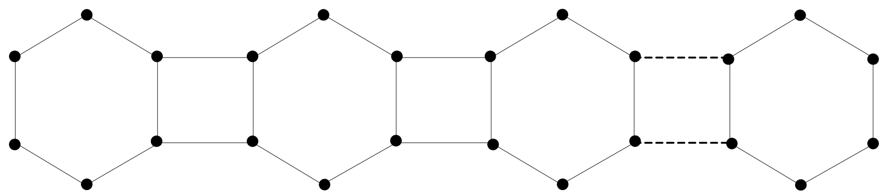

Figure 5: Linear phenylene structure of dimension n.

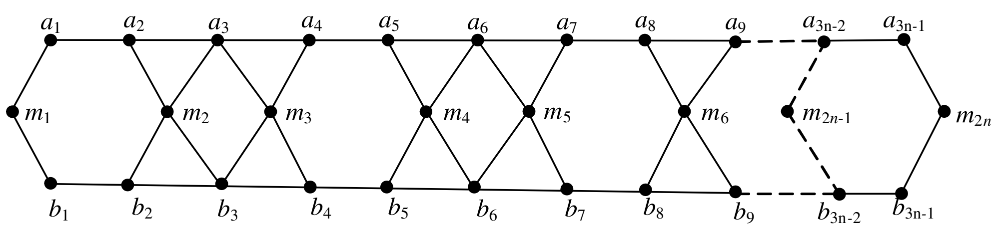

Figure 6: Labelling of the line graph of linear phenylene structure of dimension n.

This section establishes the metric dimension of the line graph for linear phenylene structure of dimension n, $n \geq 2$.

Theorem 4.1. *Let G be a linear phenylene structure of dimension n, $n \geq 2$ then $dim(L(G)) = 2$.*

Proof. Since $L(G)$ is not a path, $dim(L(G)) \geq 2$. Let $W = \{a_1, a_{3n-1}\}$ be a locating set of G. Then the identification of the vertices a_j, m_j, and b_j with respect to W are given by

$$r(a_j|W) = \{ \ (j-1, 3n-j-1) \quad \text{for all } j,\ 1 \leq j \leq 3n-1,$$

$$r(m_j|W) = \begin{cases} (j, 3n-1), & \text{if } j = 1\ , \\ (j, 3n-3), & \text{if } j = 2\ , \\ (j, 3n-4), & \text{if } j = 3\ , \\ (\frac{3j-2}{2}, \frac{6n-3j}{2}), & \text{if } 4 \leq j \leq 2n-4 \textit{ and } j \textit{ is even}, \\ (\frac{3j-3}{2}, \frac{6n-3j+1}{2}), & \text{if } 5 \leq j \leq 2n-3 \textit{ and } j \textit{ is odd}, \\ (3n-4, 3), & \text{if } j = 2n-2\ , \\ (3n-3, 2), & \text{if } j = 2n-1\ , \\ (3n-1, 1), & \text{if } j = 2n, \end{cases}$$

and

$$r(b_j|W) = \begin{cases} (2, 3n-1), & \text{if } j = 1\ , \\ (3, 3n-2), & \text{if } j = 2\ , \\ (j, 3n-j), & \text{if } 3 \leq j \leq 3n-3\ , \\ (3n-2, 3), & \text{if } j = 3n-2\ , \\ (3n-1, 2), & \text{if } j = 3n-1. \end{cases}$$

It is clear that every vertex of $L(G)$ has a unique representation with regard to W. Hence $dim((L(G)) = 2$. ■

For illustration, the line graph of the linear phenylene structure of dimension 3 is given in Figure 7.

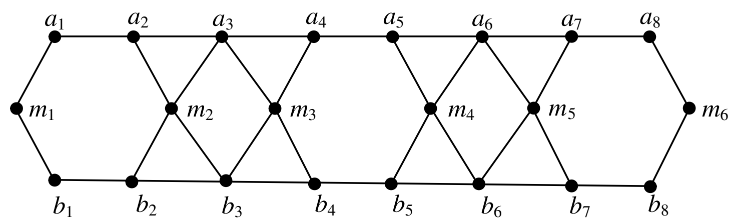

Figure 7: Labelling of the line graph of the linear phenylene structure of dimension 3.

As per Theorem 4.1, let us consider the resolving set $W = \{a_1, a_8\}$. Now, the representation of all the points with respect to W is given as follows:
$r(a_1|W) = (0, 7)$, $r(a_2|W) = (1, 6)$, $r(a_3|W) = (2, 5)$, $r(a_4|W) = (3, 4)$, $r(a_5|W) = (4, 3)$, $r(a_6|W) = (5, 2)$, $r(a_7|W) = (6, 1)$, $r(a_8|W) = (7, 0)$. Similarly, $r(m_1|W) = (1, 8)$, $r(m_2|W) = (2, 6)$, $r(m_3|W) = (3, 5)$, $r(m_4|W) = (5, 3)$, $r(m_5|W) = (6, 2)$, $r(m_6|W) = (8, 1)$, and $r(b_1|W) = (2, 8)$, $r(b_2|W) = (3, 7)$, $r(b_3|W) = (3, 6)$, $r(b_4|W) = (4, 5)$, $r(b_5|W) = (5, 4)$, $r(b_6|W) = (6, 3)$, $r(b_7|W) = (7, 3)$, $r(b_8|W) = (8, 2)$.

5 Metric dimension for line graph of linear heptagonal structure

Consider H_n as the linear heptagonal structure depicted in Figure 8, where two heptagons share two common edges. In other words, these two heptagons can be visualized as incorporating two P_2 (path graphs with two vertices) and attaching them. For heptagon applications resulting from various attributes, see [21]. The labeling of the line graph of the linear heptagonal structure is given in Figure 9. It has 5 levels, a_j, v_j, b_j, u_j, and m_j as $a_1, a_2, a_3, \ldots, a_{4n-3}, a_{4n-2}$; $v_1, v_2, v_3, \ldots, v_{4n-3}, v_{4n-2}$; $b_1, b_2, b_3, \ldots, b_n$; $u_1, u_2, u_3, \ldots, u_n$; and $m_1, m_2, m_3, \ldots, m_n$ from left to right respectively.

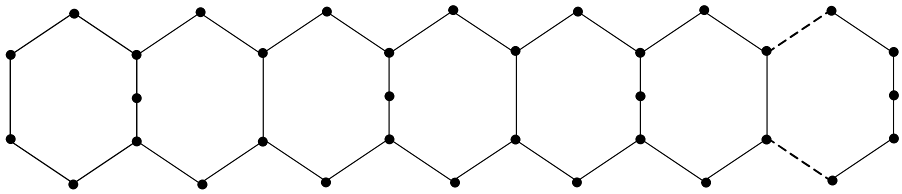

Figure 8: Linear heptagonal structure of dimension n.

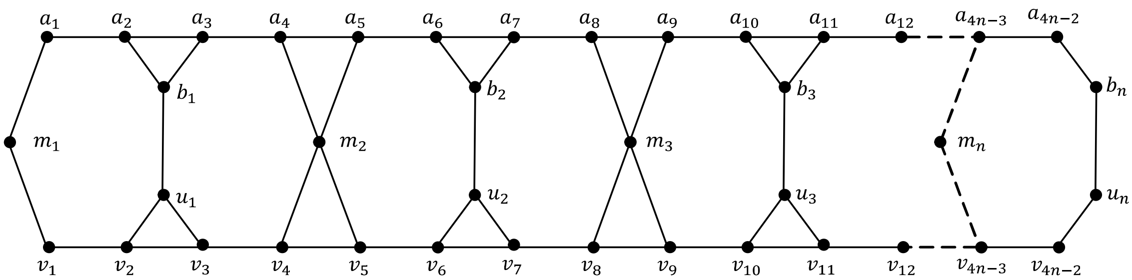

Figure 9: Labelling of the line graph of linear heptagonal structure of dimension n.

This section establishes the metric dimension of the line graph for linear heptagonal structure of dimension n, $n > 2$.

Theorem 5.1. *Let G be a linear heptagonal structure of dimension n, $n > 2$ then $dim(L(G)) = 2$.*

Proof. Since $L(G)$ is not a path, $dim(L(G)) \geq 2$. Let $W = \{a_2, a_{4n-2}\}$ be a locating set of $L(G)$. Then the identification of the vertices a_j, b_j, m_j, u_j and v_j with respect to W are given by:
For $1 \leq j \leq 4n-2$, the representation a_j of $L(G)$ with respect to W as follows:

$$r(a_j|W) = \begin{cases} (1, 4n-3), & \text{if } j = 1 \text{ ,} \\ (j-2, 4n-j-2), & \text{if } 2 \leq j \leq 4n-2 \text{ .} \end{cases}$$

For $1 \leq j \leq n$ the representation b_j of $L(G)$ with respect to W as follows:

$$r(b_j|W) = \begin{cases} (4j-3, 4n-4j), & \text{if } 1 \leq j \leq n-1 \text{ ,} \\ (4n-3, 1), & \text{if } j = n \text{ .} \end{cases}$$

For $1 \leq j \leq n$ the representation m_j of $L(G)$ with respect to W as follows:

$$r(m_j|W) = \begin{cases} (2, 4n-2), & \text{if } j = 1 \ , \\ (4j-5, 4n+2-4j), & \text{if } 2 \leq j \leq n \ . \end{cases}$$

For $1 \leq j \leq n$ the representation u_j of $L(G)$ with respect to W as follows:

$$r(u_j|W) = \begin{cases} (4j-2, 4n+1-4j), & \text{if } 1 \leq j \leq n-1 \ , \\ (4n-2, 2), & \text{if } j = n \ . \end{cases}$$

For $1 \leq j \leq 4n-2$ the representation v_j of $L(G)$ with respect to W as follows:

$$r(v_j|W) = \begin{cases} (3, 4n-1-j), & \text{if } 1 \leq j \leq 3 \ , \\ (j, 4n-5), & \text{if } j = 4 \ , \\ (j-1, 4n-1-j), & \text{if } 5 \leq j \leq 4n-5 \ , \\ (j-1, 3), & \text{if } 4n-4 \leq j \leq 4n-2 \ . \end{cases}$$

It is clear that every vertex of $L(G)$ has a unique representation with regard to W. Hence $dim((L(G)) = 2$. ■

6 Implementation and applications

In graph theory, the idea of metric dimension, particularly concerning the line graphs of cyclic hexagonal-square chains, linear phenylene structure, and linear heptagonal structures, finds application in various real-world scenarios, such as network navigation, communication networks, social network analysis, chemical and molecular structures, circuit design, and VLSI.

Network navigation: Understanding the metric dimension of these line graphs aids in designing efficient navigation strategies in various network systems. In applications such as GPS navigation, identifying the minimum set of nodes that uniquely determine the location of an object is crucial for routing and pathfinding.

Communication networks: In communication protocols and network design, determining the metric dimension helps optimize the placement of relays or information centers. Knowing the smallest set of nodes needed to monitor or control a network ensures robust communication and fault tolerance.

Social network analysis: When applied to social networks or community structures, metric dimension analysis can help identify influential individuals or key nodes whose removal may impact information flow or influence within a community.

Chemical and molecular structures: In the study of chemical compounds or molecular structures, analyzing the metric dimension of line graphs provides insights into the spatial arrangements and connectivity of atoms. This information is vital in fields like chemistry, pharmaceuticals, and material science.

Circuit design and VLSI (very large scale integration): In electronic circuit design, determining the metric dimension of line graphs helps optimize the layout of components, reducing the number of necessary connections and improving the efficiency of the overall design.

Understanding the metric dimension of line graphs in complex structures like cyclic hexagonal-square chains, linear phenylene structures, and linear heptagonal structures is not only significant within the realm of graph theory but has far-reaching implications in practical, real-world applications across diverse fields. This understanding helps in optimizing resources, improving network robustness, and advancing various technological and scientific domains.

7 Concluding remarks

In this paper, we have determined the metric dimension of the line graph for complex structures such as the cyclic hexagonal-square chain, the linear phenylene structure, and the Linear heptagonal structure, which presents a fascinating challenge in graph theory. The investigation into these structures revealed intricate patterns and relationships between vertices and their respective distances, shedding light on the fundamental properties of these graphs. The exploration of metric dimension not only enhances our understanding of these specific structures but also contributes to the broader field of graph theory, offering insights into navigation, network design, and the analysis of communication protocols in various real-world applications. Further research in this area promises to unveil deeper insights into the behavior and properties of complex graphs, paving the way for innovative solutions and advancements in diverse domains.

Conflicts of interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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